PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
PROJECT LEADER: J. B. Wooten
PERIOD COVERED: July, 1987

I. SOLUTION NMR (R. Bassfield)

A. Objective: Determine the chemical structure of flavors and odorants.

B. Results:

1. The NMR chemical shift assignments of trimethyl isoxazole were made on the basis of model compounds and a two dimensional ^{1}H-^{13}C correlation spectrum. The assignments were confirmed by measuring the ^{13}C-^{13}C satellites in the 1-D ^{13}C NMR spectrum.

2. Several two dimensional pulse sequences now exist that permit the assignment of carbon signals based on correlations of ^{1}H-^{13}C couplings over two or three bonds. These pulse sequences have been used with some success in the past, but technical problems have prevented us from using them routinely. Currently we are trying to work these problems out using l-carvone as a model case. Potentially these pulse sequences are very valuable for making structural assignments in compounds having one or more hetero atoms or non-protonated carbons.

II. NMR SERVICE (J. Campbell and S. Marrs)

A. Objective: Provide rapid NMR service to PM scientists.

B. Results:

1. Steve Marrs has installed a new probe on the XL-300 that permits both a proton and carbon spectrum to be obtained without removing the sample from the magnet. This probe should improve sample throughput for service spectra since both the proton and carbon spectra can be obtained without the need to change probes and re-shimming the magnet. A "WALTZ" modulator that significantly improves proton-carbon decoupling efficiency and minimizes sample heating problems was also installed on the XL-300.

2. A new data field for CR numbers has been created in the NMR Database and NMR data from the CR file arebeing entered into the database by John Campbell. This field will permit the NMR spectra of the well characterized chemicals in the file to be quickly located. The data in the file are being used to cross check the chemical names and formulas that have already been entered into the database.